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3,5-Bis(4-methylphenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

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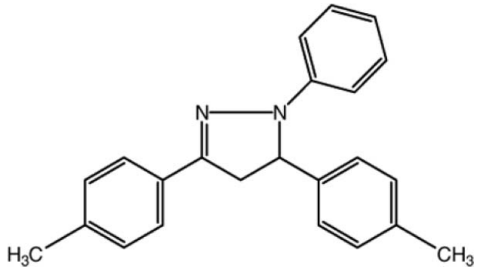
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 15.9.

In the title compound, $C_{23}H_{22}N_2$, the dihedral angle between the methylbenzene groups is 77.62 (6)°, and the dihedral angle between the envelope-shaped pyrazole ring [in which one C atom displaced by 0.109 (1) Å from the mean plane of the other four atoms] and the phenyl ring is 17.57 (7)°. The dihedral angles between the phenyl ring and the two methylbenzene rings are 13.24 (6) and 81.02 (7)°. In the crystal, weak C—H$\cdots\pi$ interactions link the molecules.

Related literature

For related structures and background references, see: Jasinski *et al.* (2010); Samshuddin *et al.* (2010).



Experimental

Crystal data

$C_{23}H_{22}N_2$
M_r = 326.43
Monoclinic, $P2_1/n$
a = 5.8113 (3) Å
b = 10.6959 (5) Å
c = 28.4455 (13) Å
β = 94.983 (4)°
V = 1761.41 (15) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 123 K
0.53 × 0.11 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini CCD diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2007)
T_{min} = 0.736, T_{max} = 1.000
12872 measured reflections
3615 independent reflections
3096 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.03
3615 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2, *Cg*3 and *Cg*4 are the centroids of the C4–C9, C10–C15 and C17–C22 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$B\cdots Cg3^{i}$	0.99	2.74	3.5766 (13)	142
C12—H12$A\cdots Cg2^{ii}$	0.95	2.69	3.5485 (15)	150
C16—H16$C\cdots Cg4^{iii}$	0.98	2.81	3.6144 (17)	140
C23—H23$B\cdots Cg4^{iv}$	0.98	2.77	3.5742 (16)	140

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5825).

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supporting information

Acta Cryst. (2011). E**67**, o1019 [doi:10.1107/S1600536811011494]

3,5-Bis(4-methylphenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

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S1. Comment

In continuation of our work on pyrazoline derivatives Samshuddin *et al.*, 2010, Jasinski *et al.*, 2010), we now describe the synthesis and structure of the title compound, (I).

The title compound (I) contains two methylbenzene groups and a phenyl ring attached to an envelope configured pyrazole ring (Fig. 1). The dihedral angle between the two methylbenzene groups is 77.62 (6)° and the dihedral angle between the pyrazole and phenyl rings is 17.57 (7)°. Also, the dihedral angles between the phenyl ring and the two methyl-substituted phenyl groups are 13.24 (6) and 81.02 (7)°, respectively. Four C–H···π interactions (Table 1) contribute to the stability of the crystal structure (Fig. 2).

S2. Experimental

A mixture of (2*E*)-1,3-bis(4-methylphenyl)prop-2-en-1-one (2.36 g, 0.01 mol) and phenyl hydrazine (1.08 g, 0.01 mol) in 50 ml glacial acetic acid was refluxed for 6 h. The reaction mixture was cooled and poured into 50 ml ice-cold water. The precipitate was collected by filtration and purified by recrystallization from ethanol. Yellow needles of (I) were grown from acetonitrile by slow evaporation (m. p.: 412–414 K, yield: 78%).

S3. Refinement

All H atoms were placed in their calculated positions (methyl C—H = 0.98 Å, methylene C—H = 0.99 Å, methine C—H = 1.00 Å and aromatic C—H = 0.95 Å) and refined using a riding model. Isotropic displacement parameters for these atoms were set to 1.2 (or 1.5 for the methyl group) times the U_{eq} of the parent atom.

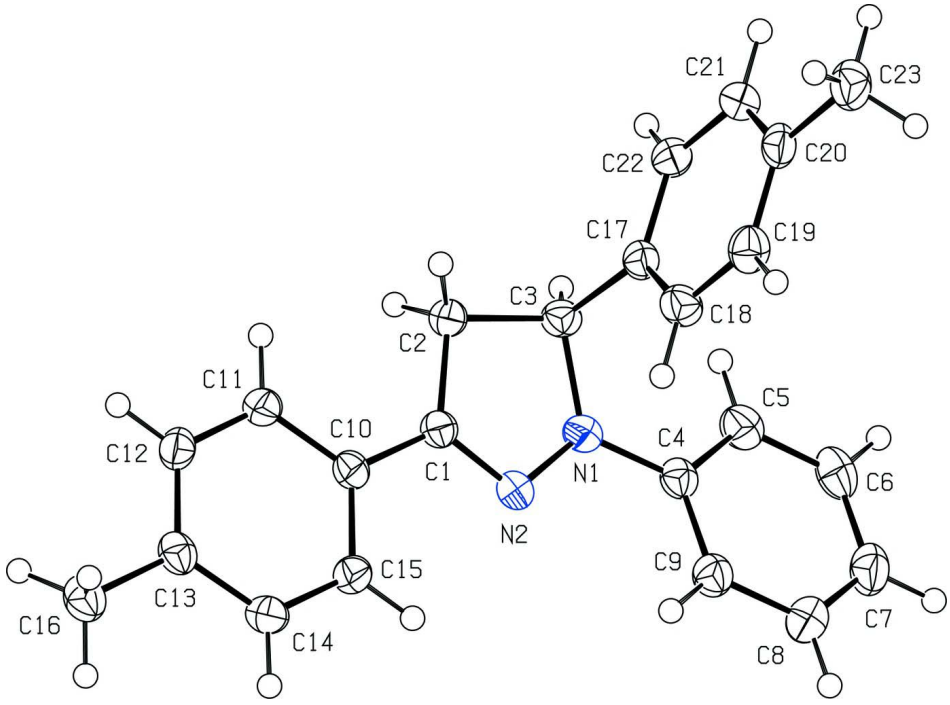

Figure 1

Molecular structure of the title compound showing displacement ellipsoids for non-H atoms drawn at the 50% probability level.

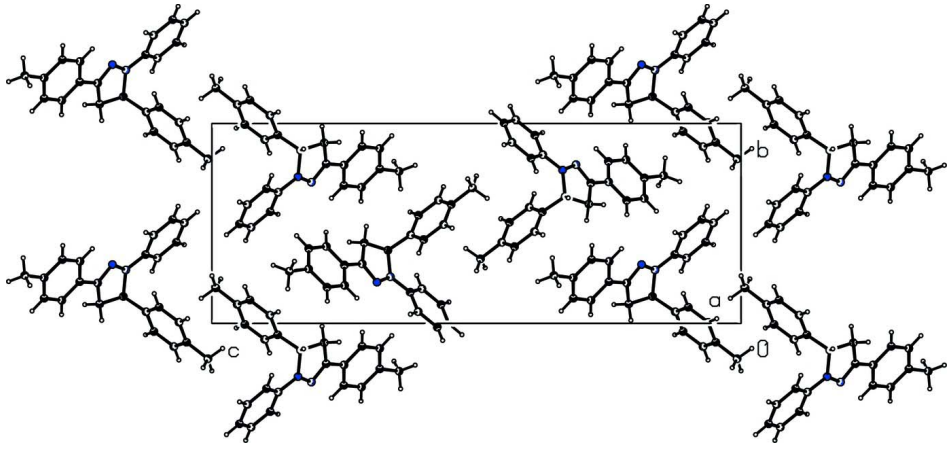

Figure 2

Packing diagram of the title compound viewed down the *a* axis.

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Crystal data

$C_{23}H_{22}N_2$
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c = 28.4455 (13) Å
β = 94.983 (4)°
V = 1761.41 (15) Å^3
Z = 4
F(000) = 696
D_x = 1.231 Mg m^{-3}

Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6406 reflections
θ = 4.4–75.5°
μ = 0.55 mm^{-1}
T = 123 K
Needle, yellow
0.53 × 0.11 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini CCD diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*;Oxford Diffraction, 2007)
T_{min} = 0.736, T_{max} = 1.000
12872 measured reflections
3615 independent reflections
3096 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 75.7°, θ_{min} = 4.4°
h = −7→6
k = −13→13
l = −34→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.03
3615 reflections
228 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.4363P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.03560 (19)	0.23302 (10)	0.66268 (4)	0.0274 (3)
N2	0.24215 (19)	0.20597 (10)	0.68799 (4)	0.0255 (3)
C1	0.2985 (2)	0.29796 (11)	0.71599 (4)	0.0246 (3)
C2	0.1238 (2)	0.40318 (12)	0.71220 (4)	0.0269 (4)
C3	−0.0306 (2)	0.36569 (12)	0.66740 (5)	0.0257 (3)
C4	−0.0433 (2)	0.15597 (12)	0.62528 (4)	0.0253 (3)
C5	−0.2649 (2)	0.17337 (14)	0.60319 (5)	0.0331 (4)
C6	−0.3486 (3)	0.09418 (15)	0.56701 (5)	0.0355 (4)
C7	−0.2145 (3)	−0.00281 (14)	0.55219 (5)	0.0380 (5)
C8	0.0064 (3)	−0.01954 (15)	0.57400 (5)	0.0374 (4)
C9	0.0931 (2)	0.05842 (13)	0.61021 (5)	0.0297 (4)
C10	0.5036 (2)	0.29188 (12)	0.74964 (4)	0.0243 (3)

C11	0.5501 (2)	0.38492 (12)	0.78377 (5)	0.0276 (4)
C12	0.7391 (2)	0.37447 (12)	0.81698 (5)	0.0282 (4)
C13	0.8878 (2)	0.27223 (12)	0.81727 (5)	0.0272 (4)
C14	0.8428 (2)	0.18087 (12)	0.78254 (5)	0.0289 (4)
C15	0.6556 (2)	0.18988 (12)	0.74930 (5)	0.0266 (4)
C16	1.0901 (3)	0.26048 (14)	0.85368 (5)	0.0342 (4)
C17	0.0167 (2)	0.44225 (12)	0.62430 (4)	0.0247 (3)
C18	0.2099 (2)	0.41944 (13)	0.59980 (5)	0.0302 (4)
C19	0.2591 (2)	0.49430 (14)	0.56221 (5)	0.0317 (4)
C20	0.1173 (3)	0.59488 (12)	0.54784 (5)	0.0294 (4)
C21	−0.0768 (3)	0.61616 (12)	0.57187 (5)	0.0314 (4)
C22	−0.1273 (2)	0.54094 (12)	0.60961 (5)	0.0285 (4)
C23	0.1766 (3)	0.67715 (14)	0.50757 (5)	0.0388 (4)
H2A	0.19920	0.48500	0.70820	0.0320*
H2B	0.03430	0.40650	0.74020	0.0320*
H3A	−0.19730	0.37210	0.67330	0.0310*
H5A	−0.35870	0.23960	0.61290	0.0400*
H6A	−0.49980	0.10670	0.55220	0.0430*
H7A	−0.27280	−0.05700	0.52750	0.0460*
H8A	0.09980	−0.08560	0.56390	0.0450*
H9A	0.24470	0.04570	0.62480	0.0360*
H11A	0.45170	0.45570	0.78420	0.0330*
H12A	0.76760	0.43840	0.83990	0.0340*
H14A	0.94320	0.11100	0.78180	0.0350*
H15A	0.62960	0.12660	0.72600	0.0320*
H16A	1.04610	0.29080	0.88410	0.0510*
H16B	1.21930	0.31040	0.84400	0.0510*
H16C	1.13670	0.17260	0.85660	0.0510*
H18A	0.30930	0.35160	0.60900	0.0360*
H19A	0.39150	0.47680	0.54600	0.0380*
H21A	−0.17720	0.68340	0.56240	0.0380*
H22A	−0.26150	0.55730	0.62540	0.0340*
H23A	0.05160	0.73740	0.50010	0.0580*
H23B	0.19620	0.62540	0.47980	0.0580*
H23C	0.32050	0.72220	0.51660	0.0580*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0281 (6)	0.0256 (5)	0.0276 (6)	0.0039 (4)	−0.0019 (4)	0.0005 (4)
N2	0.0263 (5)	0.0264 (5)	0.0234 (5)	0.0016 (4)	−0.0005 (4)	0.0017 (4)
C1	0.0293 (6)	0.0236 (6)	0.0213 (6)	0.0016 (5)	0.0049 (5)	0.0019 (4)
C2	0.0328 (7)	0.0254 (6)	0.0229 (6)	0.0042 (5)	0.0047 (5)	0.0007 (5)
C3	0.0249 (6)	0.0254 (6)	0.0270 (6)	0.0035 (5)	0.0043 (5)	0.0009 (5)
C4	0.0276 (6)	0.0256 (6)	0.0228 (6)	−0.0036 (5)	0.0028 (5)	0.0033 (5)
C5	0.0301 (7)	0.0363 (7)	0.0325 (7)	0.0025 (5)	0.0007 (5)	0.0029 (6)
C6	0.0296 (7)	0.0454 (8)	0.0301 (7)	−0.0057 (6)	−0.0047 (6)	0.0062 (6)
C7	0.0461 (9)	0.0390 (8)	0.0277 (7)	−0.0096 (6)	−0.0038 (6)	−0.0025 (6)

C8	0.0430 (8)	0.0361 (7)	0.0326 (7)	0.0022 (6)	0.0003 (6)	−0.0061 (6)
C9	0.0286 (7)	0.0318 (7)	0.0282 (7)	0.0003 (5)	−0.0002 (5)	−0.0008 (5)
C10	0.0283 (6)	0.0243 (6)	0.0206 (6)	−0.0009 (5)	0.0036 (5)	0.0032 (5)
C11	0.0341 (7)	0.0242 (6)	0.0247 (6)	0.0025 (5)	0.0040 (5)	0.0012 (5)
C12	0.0366 (7)	0.0266 (6)	0.0213 (6)	−0.0036 (5)	0.0028 (5)	−0.0014 (5)
C13	0.0292 (7)	0.0286 (6)	0.0237 (6)	−0.0043 (5)	0.0019 (5)	0.0050 (5)
C14	0.0299 (7)	0.0250 (6)	0.0316 (7)	0.0025 (5)	0.0013 (5)	0.0023 (5)
C15	0.0315 (7)	0.0229 (6)	0.0252 (6)	−0.0009 (5)	0.0020 (5)	−0.0011 (5)
C16	0.0350 (7)	0.0342 (7)	0.0320 (7)	−0.0050 (6)	−0.0044 (6)	0.0026 (6)
C17	0.0247 (6)	0.0267 (6)	0.0224 (6)	0.0011 (5)	0.0000 (5)	−0.0009 (5)
C18	0.0271 (7)	0.0344 (7)	0.0292 (7)	0.0067 (5)	0.0027 (5)	0.0020 (5)
C19	0.0290 (7)	0.0390 (7)	0.0277 (7)	−0.0002 (5)	0.0060 (5)	−0.0015 (5)
C20	0.0377 (7)	0.0288 (6)	0.0210 (6)	−0.0067 (5)	−0.0018 (5)	−0.0020 (5)
C21	0.0393 (8)	0.0260 (6)	0.0282 (7)	0.0052 (5)	−0.0017 (6)	0.0008 (5)
C22	0.0292 (7)	0.0291 (6)	0.0272 (6)	0.0051 (5)	0.0031 (5)	−0.0018 (5)
C23	0.0546 (9)	0.0354 (7)	0.0264 (7)	−0.0087 (6)	0.0034 (6)	0.0017 (6)

Geometric parameters (Å, º)

N1—N2	1.3758 (16)	C20—C21	1.388 (2)
N1—C3	1.4794 (17)	C20—C23	1.508 (2)
N1—C4	1.3916 (16)	C21—C22	1.393 (2)
N2—C1	1.2901 (16)	C2—H2A	0.9900
C1—C2	1.5132 (17)	C2—H2B	0.9900
C1—C10	1.4639 (16)	C3—H3A	1.0000
C2—C3	1.5464 (18)	C5—H5A	0.9500
C3—C17	1.5191 (18)	C6—H6A	0.9500
C4—C5	1.3955 (17)	C7—H7A	0.9500
C4—C9	1.3999 (18)	C8—H8A	0.9500
C5—C6	1.388 (2)	C9—H9A	0.9500
C6—C7	1.385 (2)	C11—H11A	0.9500
C7—C8	1.388 (2)	C12—H12A	0.9500
C8—C9	1.386 (2)	C14—H14A	0.9500
C10—C11	1.4001 (18)	C15—H15A	0.9500
C10—C15	1.4043 (18)	C16—H16A	0.9800
C11—C12	1.3896 (18)	C16—H16B	0.9800
C12—C13	1.3934 (18)	C16—H16C	0.9800
C13—C14	1.3980 (19)	C18—H18A	0.9500
C13—C16	1.503 (2)	C19—H19A	0.9500
C14—C15	1.3813 (18)	C21—H21A	0.9500
C17—C18	1.3935 (17)	C22—H22A	0.9500
C17—C22	1.3887 (18)	C23—H23A	0.9800
C18—C19	1.385 (2)	C23—H23B	0.9800
C19—C20	1.395 (2)	C23—H23C	0.9800
N2—N1—C3	112.10 (10)	H2A—C2—H2B	109.00
N2—N1—C4	119.35 (10)	N1—C3—H3A	110.00
C3—N1—C4	124.50 (11)	C2—C3—H3A	110.00

N1—N2—C1	109.02 (10)	C17—C3—H3A	110.00
N2—C1—C2	112.98 (10)	C4—C5—H5A	120.00
N2—C1—C10	121.23 (11)	C6—C5—H5A	120.00
C2—C1—C10	125.64 (10)	C5—C6—H6A	120.00
C1—C2—C3	101.74 (10)	C7—C6—H6A	120.00
N1—C3—C2	100.76 (10)	C6—C7—H7A	121.00
N1—C3—C17	112.15 (11)	C8—C7—H7A	121.00
C2—C3—C17	113.12 (10)	C7—C8—H8A	119.00
N1—C4—C5	119.68 (12)	C9—C8—H8A	119.00
N1—C4—C9	121.18 (11)	C4—C9—H9A	120.00
C5—C4—C9	119.11 (12)	C8—C9—H9A	120.00
C4—C5—C6	120.19 (13)	C10—C11—H11A	120.00
C5—C6—C7	120.84 (15)	C12—C11—H11A	120.00
C6—C7—C8	118.92 (14)	C11—C12—H12A	119.00
C7—C8—C9	121.14 (14)	C13—C12—H12A	119.00
C4—C9—C8	119.81 (12)	C13—C14—H14A	119.00
C1—C10—C11	121.26 (11)	C15—C14—H14A	119.00
C1—C10—C15	120.46 (11)	C10—C15—H15A	120.00
C11—C10—C15	118.25 (11)	C14—C15—H15A	120.00
C10—C11—C12	120.52 (11)	C13—C16—H16A	109.00
C11—C12—C13	121.35 (12)	C13—C16—H16B	109.00
C12—C13—C14	117.81 (12)	C13—C16—H16C	109.00
C12—C13—C16	121.15 (12)	H16A—C16—H16B	109.00
C14—C13—C16	121.04 (11)	H16A—C16—H16C	110.00
C13—C14—C15	121.52 (12)	H16B—C16—H16C	109.00
C10—C15—C14	120.53 (12)	C17—C18—H18A	120.00
C3—C17—C18	121.29 (11)	C19—C18—H18A	120.00
C3—C17—C22	120.40 (11)	C18—C19—H19A	119.00
C18—C17—C22	118.25 (12)	C20—C19—H19A	120.00
C17—C18—C19	120.94 (12)	C20—C21—H21A	119.00
C18—C19—C20	121.05 (12)	C22—C21—H21A	119.00
C19—C20—C21	117.84 (13)	C17—C22—H22A	120.00
C19—C20—C23	120.31 (14)	C21—C22—H22A	120.00
C21—C20—C23	121.85 (13)	C20—C23—H23A	110.00
C20—C21—C22	121.30 (13)	C20—C23—H23B	109.00
C17—C22—C21	120.61 (12)	C20—C23—H23C	110.00
C1—C2—H2A	111.00	H23A—C23—H23B	109.00
C1—C2—H2B	111.00	H23A—C23—H23C	109.00
C3—C2—H2A	111.00	H23B—C23—H23C	109.00
C3—C2—H2B	111.00		

C3—N1—N2—C1	12.24 (14)	N1—C4—C9—C8	177.64 (13)
C4—N1—N2—C1	170.61 (11)	C5—C4—C9—C8	−0.4 (2)
N2—N1—C3—C2	−18.27 (13)	C4—C5—C6—C7	−0.1 (2)
N2—N1—C3—C17	102.32 (12)	C5—C6—C7—C8	−0.3 (2)
C4—N1—C3—C2	−175.32 (11)	C6—C7—C8—C9	0.3 (2)
C4—N1—C3—C17	−54.74 (15)	C7—C8—C9—C4	0.0 (2)
N2—N1—C4—C5	172.10 (12)	C1—C10—C11—C12	176.68 (12)

N2—N1—C4—C9	−5.93 (18)	C15—C10—C11—C12	−1.44 (19)
C3—N1—C4—C5	−32.39 (18)	C1—C10—C15—C14	−176.72 (12)
C3—N1—C4—C9	149.59 (12)	C11—C10—C15—C14	1.41 (19)
N1—N2—C1—C2	0.12 (14)	C10—C11—C12—C13	0.3 (2)
N1—N2—C1—C10	175.95 (10)	C11—C12—C13—C14	0.90 (19)
N2—C1—C2—C3	−11.25 (13)	C11—C12—C13—C16	−179.14 (13)
C10—C1—C2—C3	173.14 (11)	C12—C13—C14—C15	−0.93 (19)
N2—C1—C10—C11	−172.36 (12)	C16—C13—C14—C15	179.11 (13)
N2—C1—C10—C15	5.72 (18)	C13—C14—C15—C10	−0.2 (2)
C2—C1—C10—C11	2.91 (18)	C3—C17—C18—C19	−176.21 (12)
C2—C1—C10—C15	−179.01 (11)	C22—C17—C18—C19	0.94 (19)
C1—C2—C3—N1	16.33 (11)	C3—C17—C22—C21	176.07 (12)
C1—C2—C3—C17	−103.56 (11)	C18—C17—C22—C21	−1.10 (19)
N1—C3—C17—C18	−36.48 (16)	C17—C18—C19—C20	0.2 (2)
N1—C3—C17—C22	146.44 (12)	C18—C19—C20—C21	−1.1 (2)
C2—C3—C17—C18	76.66 (15)	C18—C19—C20—C23	178.58 (13)
C2—C3—C17—C22	−100.43 (13)	C19—C20—C21—C22	1.0 (2)
N1—C4—C5—C6	−177.62 (13)	C23—C20—C21—C22	−178.74 (13)
C9—C4—C5—C6	0.5 (2)	C20—C21—C22—C17	0.2 (2)

Hydrogen-bond geometry (Å, º)

Cg2, Cg3 and Cg4 are the centroids of the C4–C9, C10–C15 and C17–C22 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···*Cg*3^{i}	0.99	2.74	3.5766 (13)	142
C12—H12*A*···*Cg*2^{ii}	0.95	2.69	3.5485 (15)	150
C16—H16*C*···*Cg*4^{iii}	0.98	2.81	3.6144 (17)	140
C23—H23*B*···*Cg*4^{iv}	0.98	2.77	3.5742 (16)	140

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) −*x*, −*y*+1, −*z*+1.